

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptasel1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS	4	OCT 30	CHEMLIST enhanced with new search and display field
NEWS	5	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS	6	NOV 10	CA/CAPLUS F-Term thesaurus enhanced
NEWS	7	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS	8	NOV 20	CA/CAPLUS to MARPAT accession number crossover limit increased to 50,000
NEWS	9	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS	10	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS	11	DEC 14	WPIDS/WPINDEX/WPIX manual codes updated
NEWS	12	DEC 14	GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS	13	DEC 18	CA/CAPLUS pre-1967 chemical substance index entries enhanced with preparation role
NEWS	14	DEC 18	CA/CAPLUS patent kind codes updated
NEWS	15	DEC 18	MARPAT to CA/CAPLUS accession number crossover limit increased to 50,000
NEWS	16	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS	17	DEC 27	CA/CAPLUS enhanced with more pre-1907 records
NEWS	18	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS	19	JAN 16	CA/CAPLUS Company Name Thesaurus enhanced and reloaded
NEWS	20	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS	21	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS	22	JAN 22	CA/CAPLUS updated with revised CAS roles
NEWS	23	JAN 22	CA/CAPLUS enhanced with patent applications from India
NEWS	24	JAN 29	PHAR reloaded with new search and display fields
NEWS	25	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS	26	FEB 13	CASREACT coverage to be extended
NEWS	27	Feb 15	PATDPASPC enhanced with Drug Approval numbers
NEWS	28	Feb 15	RUSSIAPAT enhanced with pre-1994 records
NEWS	29	Feb 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS	30	Feb 26	MEDLINE reloaded with enhancements
NEWS	31	Feb 26	EMBASE enhanced with Clinical Trial Number field
NEWS	32	Feb 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS	33	Feb 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS	34	Feb 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

NEWS IPC8. For general information regarding STN implementation of IPC 8
NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 12:01:45 ON 12 MAR 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 12:01:56 ON 12 MAR 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 MAR 2007 HIGHEST RN 926007-42-3

DICTIONARY FILE UPDATES: 11 MAR 2007 HIGHEST RN 926007-42-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

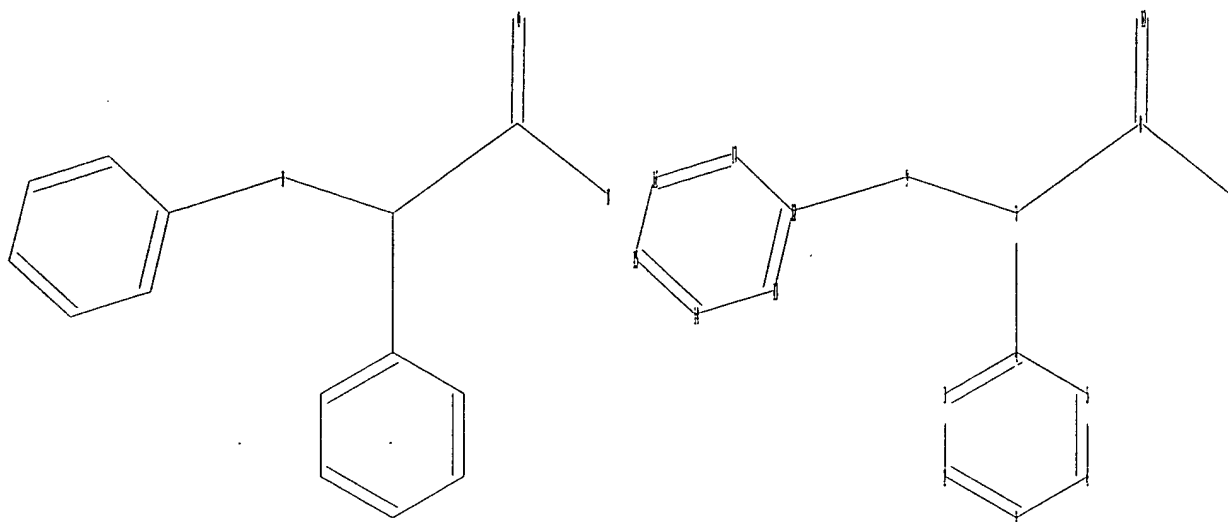
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10501932.str



chain nodes :

7 8 9 10 11

ring nodes :

1 2 3 4 5 6 12 13 14 15 16 17

chain bonds :

4-7 7-8 7-9 8-10 8-11 9-12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17

exact/norm bonds :

7-9 8-10 8-11 9-12

exact bonds :

4-7 7-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17

Match level :

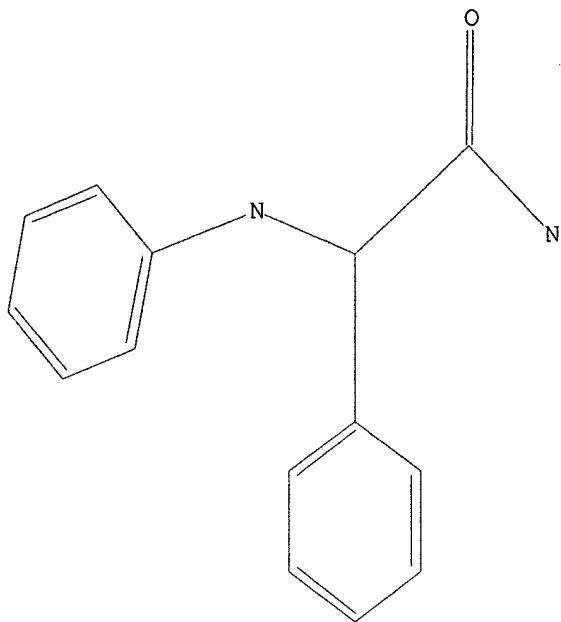
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 12:02:08 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 227 TO ITERATE

100.0% PROCESSED 227 ITERATIONS 50 ANSWERS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 3637 TO 5443
 PROJECTED ANSWERS: 2318 TO 3802

L2 50 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 12:02:14 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 4604 TO ITERATE

100.0% PROCESSED 4604 ITERATIONS 3078 ANSWERS
 SEARCH TIME: 00.00.01

L3 3078 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	172.31

FILE 'CAPLUS' ENTERED AT 12:02:16 ON 12 MAR 2007
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is

held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 12 Mar 2007 VOL 146 ISS 12
FILE LAST UPDATED: 11 Mar 2007 (20070311/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l3

L4 340 L3 .

=> s l3 and factor x

340 L3

1023681 FACTOR

924287 FACTORS

1613966 FACTOR

(FACTOR OR FACTORS)

1578035 X

4457 FACTOR X

(FACTOR(W)X)

L5 1 L3 AND FACTOR X

=> d ibib abs hitstr tot

L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:313015 CAPLUS

DOCUMENT NUMBER: 145:241095

TITLE: Effect of MCM09, an active site-directed inhibitor of factor Xa, on B16-BL6 melanoma lung colonies in mice
Rossi, C.; Hess, S.; Eckl, W.; Di Lena, A.; Bruno, A.;

AUTHOR(S): Thomas, O.; Poggi, A.
CORPORATE SOURCE: Consorzio Mario Negri Sud, Santa Maria Imbaro, Italy
SOURCE: Journal of Thrombosis and Haemostasis (2006), 4(3), 608-613

CODEN: JTHOAS; ISSN: 1538-7933

PUBLISHER: Blackwell Publishing, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Treatment with anticoagulant drugs has shown potential inhibitory effect on tumor invasion, although the relationship with clotting inhibition was not clear. The aim of our study was to evaluate the potential antitumor activity of MCM09, a newly developed, active site-directed, small mol. inhibitor of factor Xa (FXa) [W00216312], and to relate the findings to anticlotting potency. MCM09 (0.1-10 mg kg⁻¹) or heparin (H; 10 mg kg⁻¹) was injected i.v., with 5 × 10⁴ B16-BL6 melanoma cells, in C57BL/6 mice. Mice were killed after 18 days, to count lung colonies. Ex vivo anticoagulant activity was measured by activated partial thromboplastin time (APTT) on mouse plasma. MCM09, a selective inhibitor of FXa (IC₅₀

2.4 nM against human FXa), inhibited in a dose-dependent manner B16-BL6 melanoma lung colonies in mice. Mean lung metastasis number was 20.9 ± 4.8 in controls (n = 10), 1.2 ± 0.4 in mice treated with H, 10 mg kg⁻¹ i.v. (P < 0.01), 0.9 ± 0.3, 9.2 ± 2.2 and 15.5 ± 2.6 in mice treated with MCM09, at 10 (P < 0.01), 1 (P < 0.05) and 0.1 mg kg⁻¹ i.v. (ns), resp. MCM09 (10 mg kg⁻¹ i.v.) significantly prolonged APTT (57.1 ± 10.2 s) 30 min after i.v. injection when compared with controls (25.3 ± 1.6 s; P < 0.05). Lung colonies were 74.2-72.6% reduced by MCM09 (10 mg kg⁻¹) given 60 or 120 min before cells, but not by MCM09 given 60 min thereafter, suggesting a direct cell interaction as a mechanism

underlying

antitumor activity.

IT 905914-23-0

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

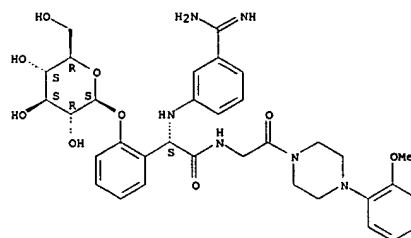
(MCM09, selective inhibitor of factor Xa inhibited dose-dependent manner B16-BL6 melanoma lung colonies, thrombin, kallikrein, protease-I, plasmin, activated protein C activity and showed total anticoagulant effect in murine model)

RN 905914-23-0 CAPLUS

CN Benzeneacetamide, α-[[3-[(aminoiminomethyl)phenyl]amino]-2-(β-D-glucopyranosyloxy)-N-[2-[4-(2-methoxyphenyl)-1-piperazinyl]-2-oxoethyl]-, (aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

```
=> s l3 and cancer
      340 L3
      308489 CANCER
      45229 CANCERS
      320112 CANCER
              (CANCER OR CANCERS)
L6      6 L3 AND CANCER

=> d ibib abs hitstr tot
```

L6 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 2004:1029049 CAPLUS
DOCUMENT NUMBER: 142:171684
TITLE: Small Molecule Modulators of Endogenous and Co-chaperone-stimulated Hsp70 ATPase Activity
AUTHOR(S): Fewell, Sheara W.; Smith, Christine M.; Lyon, Michael A.; Dumitrescu, Teodora Pene; Wipf, Peter; Day, Billy W.; Brodsky, Jeffrey L.
CORPORATE SOURCE: Department of Biological Sciences, University of Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of Biological Chemistry (2004), 279(49), 51131-51140
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:171684

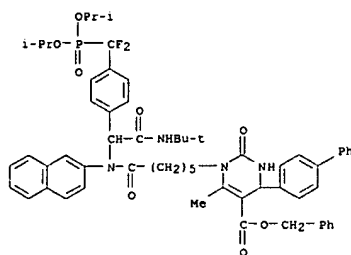
AB The mol. chaperone and cytoprotective activities of the Hsp70 and Hsp40 chaperones represent therapeutic targets for human diseases such as cancer and those that arise from defects in protein folding; however, very few Hsp70 and no Hsp40 modulators have been described. Using an assay for ATP hydrolysis, we identified and screened small mol. with structural similarity to 15-deoxyspergualin and NSC 630668-R/1 for their effects on endogenous and Hsp40-stimulated Hsp70 ATPase activity. Several of these compds. modulated Hsp70 ATPase activity, consistent with the action of NSC 630668-R/1 observed previously (Fewell, S. W., Day, B.

W., and Brodsky, J. L. (2003) J. Biol. Chemical 276, 910-914). In contrast, three compds. inhibited the ability of Hsp40 to stimulate Hsp70 ATPase activity but did not affect the endogenous activity of Hsp70. Two of these agents also compromised the Hsp70/Hsp40-mediated post-translational translocation of a secreted pre-protein in vitro. Together, these data indicate the potential for continued screening of small mol. Hsp70 effectors and that specific modulators of Hsp70-Hsp40 interaction can be obtained, potentially for future therapeutic use.

IT 831217-38-0P
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (small mol. modulators of endogenous and Hsp40-stimulated Hsp70 ATPase activity and interactions)

RN 831217-38-0 CAPLUS
CN 5-Pyrimidin-2-carboxylic acid, 4-[1,1'-biphenyl]-4-yl-1-[6-[[1,4-[[bis(1-methylethoxy)phosphinyl]difluoromethyl]phenyl]-2-[(1,1-dimethyl-2-ethoxyamino)-2-oxoethyl]-2-naphthalenylamino]-6-oxohexyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-, phenylmethyl ester (9CI) (CA INDEX NAME)

L6 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)



REFERENCE COUNT: 84 THERE ARE 84 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L6 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 2004:534173 CAPLUS
DOCUMENT NUMBER: 141:89016
TITLE: Preparation of benzimidazolylazabicyclooctylethylpiperidine
INVENTOR(S): s as Ccr5 antagonists for the treatment of HIV infection
Kazmierski, Wieslaw Mieczyslaw; Aquino, Christopher Joseph; Bifulco, Neil; Boros, Eric Eugene; Chauder, Brian Andrew; Chong, Pek Yoke; Duan, Maosheng; Deanda, Felix, Jr.; Koble, Cecilia Suarez; McLean, Ed Williams; Peckham, Jennifer Poole; Perkins, Angilique C.; Thompson, James Benjamin; Vanderwall, Dana Smithline Beecham Corporation, USA; et al.; et al.
PATENT ASSIGNEE(S): PCT Int. Appl., 859 pp.
SOURCE: CODEN: PIXKDD
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004054974	A2	20040701	WO 2003-US39644	20031212
WO 2004054974	A3	20040902		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GM, GR, GU, HK, HU, ID, IL, IN, JP, KE, KG, KP, KR, KZ, LC, LR, LS, LT, LU, LV, MA, MD, ME, MG, MK, MN, MW, MX, MY, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2509711	A1	20040701	CA 2003-2509711	20031212
AU 2003300902	A1	20040709	AU 2003-300902	20031212
EP 1569646	A2	20050907	EP 2003-813419	20031212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003017230	A	20051025	BR 2003-17230	20031212
CN 1744899	A	20060308	CN 2003-80109628	20031212
JP 2006111554	T	20060406	JP 2004-560838	20031212
NO 2005002739	A	20050819	NO 2005-2739	20050607
US 2006229336	A1	20061012	US 2005-538144	20050609
IN 2005KN01328	A	20060630	IN 2005-KN1328	20050711
PRIORITY APPLN. INFO.: US 2002-433634P P 20021213				
WO 2003-US39644 W 20031212				

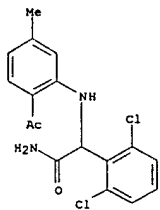
OTHER SOURCE(S): MARPAT 141:89016
GI

L6 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)

carboxyl; R2 = H, (optionally substituted) alkyl, aryl, heteroaryl, cycloalkyl, heterocycloalkyl, aralkyl, heteroarylalkyl, heteroarylalkyl, heteroarylalkyl, heteroarylsulfinyl; R3 = H, halo, cyano, trifluoromethyl, (optionally substituted) amino, acylamino, alkyl; X = C1-5 alkylene, optionally substituted with oxo or thio groups or halogen atoms, and optionally contg. 1-3 oxygen, nitrogen, sulfur, or phosphorus atoms; Y = carbonyl, thiocarbonyl, 1,2-dioxoethylene, oxyalkylcarbonyl, sulfinyl, sulfonyl, oxycyanomino, (optionally substituted) aminocarbonyl, carbonylamino, aminothiocarbonyl, oxymino, thioimino, amino, cyano, imino, methoxy, (cyanoimino)methyl, amino, (cyanoimino)methyl, amino, (sulfonylimino)methyl, amino, (sulfonylimino)methyl, amino, (alkoxyimino)methyl, amino, (imino)methyl, (cyanoimino)methoxy, iminomethoxy, (cyanoimino)methanethoxy, alkylcarbonyloxy; A = satd., partially satd., or arom. monocyclic ring with 5-6 atoms or a bicyclic ring with 8-10 members contg. 0-5 nitrogen, oxygen, and/or sulfur atoms such as II are prepd. I are prepd. as Ccr5 antagonists for the treatment of viral infections, (particularly HIV infection), related syndromes such as AIDS-related complex (ARC), progressive generalized lymphadenopathy, Kaposi's sarcoma, and neurol. conditions, and other diseases such as multiple sclerosis, rheumatoid arthritis, Crohn's disease, and immune-mediated disorders. The invention compds. have pIC50 values of 25 in assays for Ccr5 antagonism. Piperidineacetaldehyde III is prepd. in four steps from 4-phenyl-4-piperidinecarboxitrile by protection of the piperidine with Boc anhydride, reduct. of the nitrile with diisobutylaluminum hydride, Wittig olefination with methoxymethylphosphonium chloride, and hydrolysis of the enol ether with catalytic p-toluenesulfonic acid monohydrate. The hydrochloride of endo-(benzimidazolyl)azabicyclooctane IV is prepd. in five steps from tert-Bu endo-3-oxo-8-azabicyclo[3.2.1]octane-8-carboxylate; reductive amination with benzylamine, reductive cleavage of the benzyl group by palladium-mediated hydrogenation, a nucleophilic aryl substitution reaction with 1-fluoro-2-nitrobenzene, reduct. of the nitro group by hydrogenation over palladium on carbon, and treatment with tri-Et orthoacetate followed by treatment with hydrochloric acid in ethanol. Coupling of III and IV by reductive amination with sodium triacetoxymethylborohydride, cleavage of the Boc group with hydrochloric acid in dioxane, and acylation with pivaloyl chloride and triethylamine yields II. IT 147362-57-0, Loviride
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (therapeutic agents used in conjunction with benzimidazolylazabicyclooctylethylpiperidine Ccr5 antagonists in the treatment of bacterial and viral infections, particularly HIV infection, and other diseases)
RN 147362-57-0 CAPLUS
CN Benzeneacetamide, α -(2-acetyl-5-methylphenyl)amino]-2,6-dichloro-(9CI) (CA INDEX NAME)

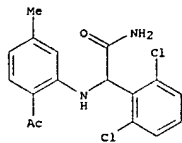
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I [R1 = (optionally substituted) alkyl, aryl, heteroaryl,



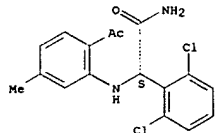
RN 141030-54-8 CAPLUS
CN Benzeneacetamide, α -[(2-acetyl-5-methylphenyl)amino]-2,6-dichloro-, (+)- (9CI) (CA INDEX NAME)

Rotation (+).



RN 141030-55-9 CAPLUS
CN Benzeneacetamide, α -[(2-acetyl-5-methylphenyl)amino]-2,6-dichloro-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



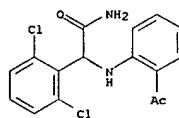
RN 147362-55-8 CAPLUS
CN Benzeneacetamide, 2,6-dichloro- α -[(2-nitrophenyl)amino]-, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

L6 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:49278 CAPLUS
DOCUMENT NUMBER: 139:159419
TITLE: Novel pharmacophore-based methods reveal gossypol as a reverse transcriptase inhibitor
AUTHOR(S): Keller, Paul A.; Birch, Chris; Leach, Scott P.; Tyssen, David; Griffith, Renate
CORPORATE SOURCE: Department of Chemistry, University of Wollongong, Wollongong, NSW 2522, Australia
SOURCE: Journal of Molecular Graphics & Modelling (2003), 21(5), 365-373
CODEN: JMGHFI; ISSN: 1093-3263
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In a program to identify new structural entities for the inhibition of the

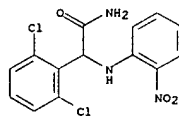
HIV-1 reverse transcriptase (RT) enzyme via database searching, a series of RT pharmacophores were developed. By utilizing a novel filtering technique, the National Cancer Institute database of compounds was scanned producing 15 compounds to be screened for activity. A notable inclusion was a series of gossypol derivatives. The testing of a series of compounds revealed the parent compound gossypol to be an HIV-1 reverse transcriptase inhibitor. These results suggest that at least a part of its anti-HIV activity is due to gossypol targeting the non-nucleoside inhibitor binding pocket of RT.
IT 141030-32-2 141030-34-4 141030-54-8
141030-55-9 147362-55-8 147362-56-9
RL: DWA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel pharmacophore-based methods reveal gossypol as a reverse transcriptase inhibitor)
RN 141030-32-2 CAPLUS
CN Benzeneacetamide, α -[(2-acetylphenyl)amino]-2,6-dichloro-, (-)- (9CI) (CA INDEX NAME)

Rotation (-).



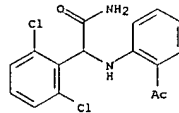
RN 141030-34-4 CAPLUS
CN Benzeneacetamide, 2,6-dichloro- α -[(2-nitrophenyl)amino]-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 147362-56-9 CAPLUS
CN Benzeneacetamide, α -[(2-acetylphenyl)amino]-2,6-dichloro-, (+)- (9CI) (CA INDEX NAME)

Rotation (+).



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L6 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 2002:869219 CAPLUS
 DOCUMENT NUMBER: 137:363028
 TITLE: Drug screening assays and kits for discovery of anti-microbial and chemotherapeutics agents
 INVENTOR(S): McCarthy, Lawrence; Kong, Lilly; Shao, Tang; Su, Xin
 PATENT ASSIGNEE(S): Focus Technologies, Inc., USA
 SOURCE: PCT Int. Appl., 94 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002090993	A2	20021114	WO 2001-US44783	20011127
WO 2002090993	A3	20040415		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2430201	A1	20021114	CA 2001-2430201	20011127
US 2003039957	A1	20030227	US 2001-996187	20011127
EP 1435000	A2	20040707	EP 2001-273944	20011127
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2005500022	T	20050106	JP 2002-588199	20011127
PRIORITY APPLN. INFO.:			US 2000-253150P	P 20001127
			US 2001-304533P	P 20010709
			US 2001-297686P	P 20010712
			US 2001-996187	A2 20011127
			WO 2001-US44783	W 20011127

AB Methods and compns. for detecting the phenotype of a bioactive mol. assays. More specifically, are provided methods and compns. are provided for determining the suitability of one or more candidate compds. prior to or

during the course of chemotherapy or anti-infective therapy, for their capacity to inhibit the bioactive mol. of micro-organisms, cancers and as an assay for expression in transgene therapy. Also provided are phenotypic assays for drug discovery. Claimed sequences were

not present at the time of publication.

IT 147362-57-0, Loviride
 RL: BSU (Biological study, unclassified); BIOL (Biological study); (drug screening assays for discovery of anti-microbial and chemotherapeutics agents)

RN 147362-57-0 CAPLUS
 CN Benzeneacetamide, α -[(2-acetyl-5-methylphenyl)amino]-2,6-dichloro-(9CI) (CA INDEX NAME)

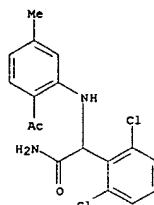
L6 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 2002:408648 CAPLUS
 DOCUMENT NUMBER: 137:6176
 TITLE: Preparation of aromatic acid derivatives useful as serine protease inhibitors
 INVENTOR(S): Bisacchi, Gregory S.; Sutton, James C., Jr.; Slusarchyk, William A.; Treuner, Uwe D.; Zhao, Guohua;
 PATENT ASSIGNEE(S): Cheney, Daniel L.; Wu, Shung C.; Shi, Yan
 SOURCE: Bristol-Myers Squibb Company, USA
 PCT Int. Appl., 182 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

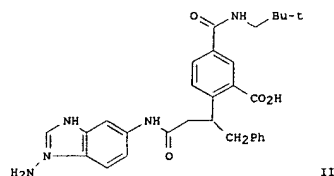
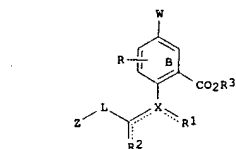
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002042273	A2	20020530	WO 2001-US46884	20011107
WO 2002042273	A3	20020829		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2428191	A1	20020530	CA 2001-2428191	20011107
AU 2002027269	A5	20020603	AU 2002-27269	20011107
EP 1332131	A2	20030806	EP 2001-996145	20011107
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2004514669	T	20040520	JP 2002-544409	20011107
HU 200400651	A2	20040628	HU 2004-651	20011107
PRIORITY APPLN. INFO.:			US 2000-246392P	P 20001107
			WO 2001-US46884	W 20011107

OTHER SOURCE(S): MARPAT 137:6176
 GI

L6 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)



L6 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)



AB Aromatic compds. I, are useful as serine protease inhibitors, wherein ring B is Ph or pyridyl; W is amide, alkyl, alkenyl, heterocycle, heteroaryl, aryl, cycloalkyl; L is a linker group; X is N, CH, or C, provided that X is C when R1 and R2 join to form a fully unsatd. ring; Z is an optionally-substituted monocyclic or bicyclic ring system; R is H, alkoxy, amine, alkyl, alkenyl, halogen, haloalkyl, cyano, nitro, alkylthio, CHO, acyl, CO2H, alkoxycarbonyl, sulfonamido, sulfonyl, Ph; R1 and R2 (i) are independently selected from hydrogen, alkyl, alkenyl, heteroaryl, aryl, heterocycle, and cycloalkyl; or (ii) are taken together to form an aryl, heteroaryl, cycloalkyl, or heterocycle, provided that R1 and R2 do not together form pyrazole when W is methoxy and Z is biphenyl; and when R1 and R2 individually or together form a heteroaryl, aryl, heterocycle, cycloalkyl; R3 is hydrogen, alkyl, substituted alkyl, heteroaryl, aryl, heterocycle, cycloalkyl, or alkyl substituted with -OC(O)R4 or -OC(O)OR4, wherein R4 is alkyl, cycloalkyl, provided that R3 is not Ph when W is methoxy. Thus, II was prepared for treating a coagulation-associated disorder,

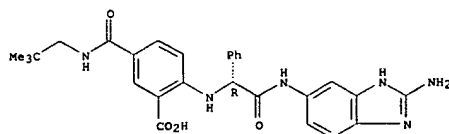
an inflammatory or immune disease, or metastases (no data). Included within the scope of the invention are pharmaceutical compns. for treating a serine protease disease, an inflammatory or immune condition, or cancer.

IT 431052-55-OP
 RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);

THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of aromatic acid derivs. useful as anti-inflammatory, anticoagulant, antitumor, immunomodulator agents and serine protease inhibitors)

L6 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RN 431052-55-0 CAPLUS
 CN Benzoic acid, 2-[[[(1R)-2-[(2-amino-1H-benzimidazol-5-yl)amino]-2-oxo-1-phenylethyl]amino]-5-[[[(2,2-dimethylpropyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

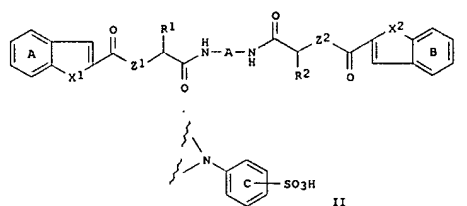
Absolute stereochemistry.



L6 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1999:640836 CAPLUS
 DOCUMENT NUMBER: 131:267038
 TITLE: Protein-carbohydrate binding antagonists
 INVENTOR(S): Herlihy, Walter C.; Rusche, James R.; Marchionni, Mark
 PATENT ASSIGNEE(S): A. Repligen Corp., USA; Cambridge Neuroscience, Inc.
 SOURCE: PCT Int. Appl., 54 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9950246	A1	19991007	WO 1999-US6792	19990329
W: .AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9933688	A	19991018	AU 1999-33688	19990329
PRIORITY APPLN. INFO.:			US 1998-32494	A 19980330
			WO 1999-US6792	W 19990329

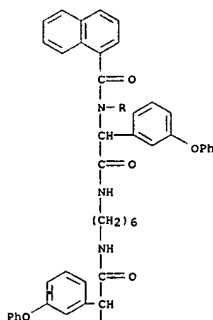
OTHER SOURCE(S): MARPAT 131:267038
 GI



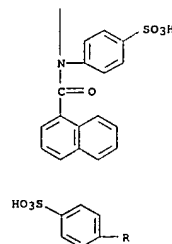
AB Comps. I (X1, X2 = NH, O, S, C:C; Z1, Z2 = O, II: A = linking group; R1, R2 = (substituted) Ph, (substituted) cyclohexyl, etc.), and physiol. acceptable salts thereof, are disclosed. The benzene rings in I and II also may be substituted. Also disclosed is a method of inhibiting binding of glycosaminoglycans with proteins whose activity is modulated by the

L6 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 glycosaminoglycans in a subject in need of such treatment. The method comprises administering to the subject an effective amt. of at least one compd. of the invention. A method for treating an erbB receptor- EGFR receptor-expressing cancer using a compd. of the invention is also disclosed.
 IT 245120-94-9P 245120-96-1P 245120-98-3P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (protein-carbohydrate binding antagonists)
 RN 245120-94-9 CAPLUS
 CN Benzenesulfonic acid, 4,4'-[[1,6-hexanediylbis(imino[2-oxo-1-(3-phenoxyphenyl)-2,1-ethanediyl] [(1-naphthalenylcarbonyl)imino]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A

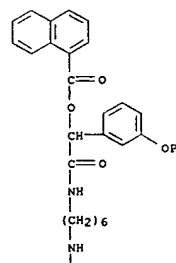


L6 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 PAGE 2-A

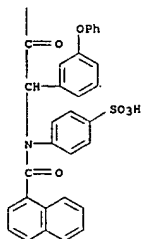


RN 245120-96-1 CAPLUS
 CN 1-Naphthalenecarboxylic acid, 2-[[[6-[[[(1-naphthalenylcarbonyl)(4-sulphophenyl)amino](3-phenoxyphenyl)acetyl]amino]hexyl]amino]-2-oxo-1-(3-phenoxyphenyl)ethyl ester (9CI) (CA INDEX NAME)

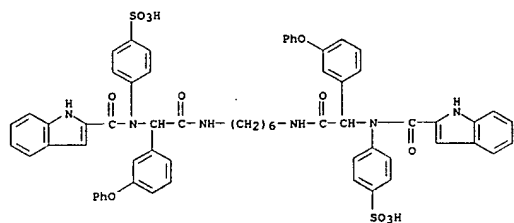
PAGE 1-A



PAGE 2-A



RN 245120-98-3 CAPLUS
 CN Benzenesulfonic acid, 4,4'-[1,6-hexanediylbis(imino[2-oxo-1-(3-phenoxyphenyl)-2,1-ethanediyl][(1H-indol-2-ylcarbonyl)imino]]bis- (9CI)
 (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

44.33

216.64

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-5.46

-5.46

STN INTERNATIONAL LOGOFF AT 12:04:01 ON 12 MAR 2007